AD NUMBER

AD820700

NEW LIMITATION CHANGE

TO

Approved for public release, distribution unlimited

FROM

Distribution authorized to U.S. Gov't. agencies and their contractors; Critical Technology; MAY 1963. Other requests shall be referred to Commander, Air Force Weapons Laboratory, Attn: WLRT, Kirtland AFB, NM 87117.

AUTHORITY

AFWL ltr, 30 Nov 1971

RTD (WLR) TM-63-2

[redacted]

A SUBROUTINE FOR THE EQUATION OF STATE OF AIR

by

L. R. Doan
1/Lt USAF

G. H. Nickel
1/Lt USAF

May 1963

TECHNICAL MEMORANDUM NUMBER RTD (WLR) TM-63-2

Research and Technology Division
Air Force Systems Command
AIR FORCE WEAPONS LABORATORY
Kirtland Air Force Base
New Mexico

Project No. 7811, Task No. 781102

HEADQUARTERS
AIR FORCE SPECIAL WEAPONS CENTER
Air Force Systems Command
Kirtland Air Force Base
New Mexico

When Government drawings, specifications, or other data are used for any purpose other than in connection with a definitely related Government procurement operation, the United States Government thereby incurs no responsibility nor any obligation whatsoever; and the fact that the Government may have formulated, furnished, or in any way supplied the said drawings, specifications, or other data, is not to be regarded by implication or otherwise as in any manner licensing the holder or any other person or corporation, or conveying any rights or permission to manufacture, use, or sell any patented invention that may in any way be related thereto.

This report is made available for study upon the understanding that the Government's proprietary interests in and relating thereto shall not be impaired. In case of apparent conflict between the Government's proprietary interests and those of others, notify the Staff Judge Advocate, Air Force Systems Command, Andrews AF Base, Washington 25, DC.

This report is published for the exchange and stimulation of ideas; it does not necessarily express the intent or policy of any higher headquarters.

Copies of th lection.
Address all req B, N Mex.

This document is subject to special export controls and each transmittal to foreign governments or foreign nationals may be made only with prior approval of Air Force Weapons Laboratory, Attn: NLRT, Kirtland AFB, New Mexico 87117.

ABSTRACT

A "semi-physical fit" to the equation of state of air is generated from tabulated values. The form is

$$P = (\gamma - 1)\,\rho\,\varepsilon$$

$$\gamma = \gamma(\rho, \varepsilon)$$

$$\rho = \text{mass/volume}$$

$$\varepsilon = \text{energy/mass}$$

A listing of the FORTRAN subroutine AIR is given, as well as a graph of tabulated and subroutine-computed values of $(\gamma - 1)$.

DAVID R. [illegible]
Colonel USAF
Chief, Physics Branch

1. A SUBROUTINE FOR THE EQUATION OF STATE OF AIR.

Computer calculations of expanding fireballs in the atmosphere require some form of equation of state for air which is valid over many orders of magnitude variation in density and energy. Many SHELL calculations have been made using an equation of state which appears much too simple. However, these calculations have given results for fireball growth and rise which agree amazingly well with experiments. Unfortunately, these results cannot be expected to give reliable pictures of temperature within the fireball simply because of the inadequacies in the equation of state. The distribution of temperatures within the fireball is extremely important in fireball calculations since it determines electron density. This note describes an interim effort to provide a good equation of state for computer codes.

Previous SHELL calculations have used γ_1 if $\varepsilon < \varepsilon_{ion}$, or γ_2 if $\varepsilon > \varepsilon_{ion}$, where ε_{ion} is an input value. The two values of γ were chosen before each problem by referring to the real equations of state. We decided to try a simple fit to $(\gamma-1)$ for an ideal gas equation of state, as computed by NBS.[1] The variables which define this equation of state are chosen as material density and energy density (per mass) rather than density and temperature. Hydrodynamics calculations always involve material and energy densities, and temperature is not used as an independent variable.*

The first look at possible forms for this fit was directed to the density dependence. Crossplots of $(\gamma-1)$ versus density for different energies revealed an approximate behavior of the form

*This fact rules out the use of analytic fits to the equation of state of air using temperature as an independent variable as in RAND RM-2249 by Harold Brode.

$$(\gamma-1) = \left[\gamma(\rho_o, \varepsilon) - 1\right] \left(\frac{\rho}{\rho_o}\right)^{a(\varepsilon)}$$

ρ_o = sea level density

= 1.293×10^{-3} gm/cm^3

The exponent a determines density spreading, and is zero below $\varepsilon = 1$ jerk per megagram or 10^{10} ergs per gram. Above $\varepsilon = 1$, $a(\varepsilon)$ is roughly linear in log (ε) (see figure 1). Assuming the density dependence discovered, the problem reduces to finding a fit for $\gamma(\rho_o, \varepsilon)$. The energy dependence of $(\gamma-1)$ is influenced by the dissociation of the major constituent molecules (only oxygen and nitrogen contribute much to the thermodynamic properties). There are four different "regimes" which are defined below:

I. Nothing dissociated $0 < \varepsilon < \sim 5$

II. Only oxygen dissociated $\sim 9 < \varepsilon < \sim 30$

III. Everything dissociated $\sim 50 < \varepsilon < \sim 150$

IV. Electrons contributing $\sim 150 < \varepsilon < \infty$

Each "regime" has its own energy dependence, and the thermodynamic properties of air are those of whichever "regime" represents the composition of the air. Transitions in properties are made as the composition changes.

Regimes I and II are affected primarily by the increasing occupation of vibrational and electronic levels of undissociated molecules. The energy dependence of regime III is due to increasing occupation of electronic energy levels, and regime IV is the threshold of the Fermi-Thomas description.*

Thermodynamically, $(\gamma-1)$ is the same as $2/n$, where n is the number of degrees of freedom. In a gas whose molecules or atoms have internal

*See, for instance, "LA-2124" on TFD theory.

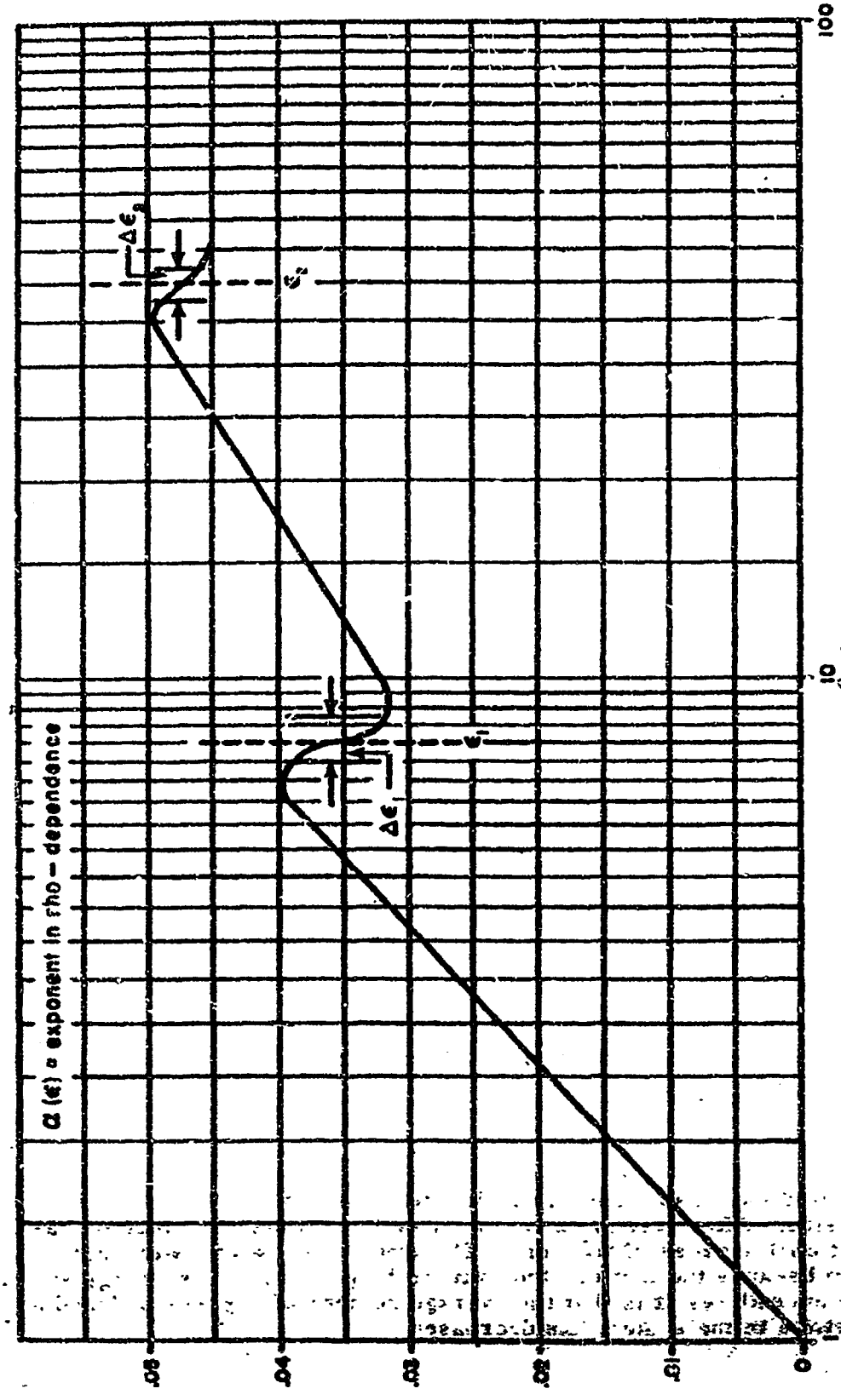


Figure 1. Sketch of α (ε) vs. ε

structure, n need not be an integer. For example, an oxygen or nitrogen molecule is rotating but not vibrating at room temperature, and has an n of 3 + 2 = 5. An energy increase will make n change from 5 to 7 (although the molecule may dissociate before n reaches 7). Regimes I and II represent this change, plus electronic excitation, for 0_2 and N_2.

The hump of increasing γ at $\varepsilon = 8$ is due to the decrease in n for oxygen from 7 to 3 as the molecules dissociate and can no longer rotate or vibrate. A similar increase in γ occurs as the nitrogen dissociates, and again as the electrons* (with no internal energy levels) become numerous.

A fit to $\gamma(\rho_o, \varepsilon)$ for the entire interval could be generated by a large polynomial, but there is more physical significance in a series of experimental fits for each regime which are "turned on and off" as the composition changes.

In practice, "on and off switches" of the form

$$f_i = \frac{1}{1 + \exp\left(\frac{\varepsilon - \varepsilon_o}{\Delta\varepsilon_o}\right)}$$

have been found to cause suitable transitions at the "humps" between functions which have been chosen to fit the data closely between "lumps." These switches have values from 0 to 1 with a certain width ($\sim 6\Delta\varepsilon$) centered about the energy ε_o and have no particular physical significance in this work. It seems reasonable to suppose, however, that ε_o is related in some way to the dissociation energy and $\Delta\varepsilon$ to the dissociation equilibrium constant.

*An excited atom has many available energy states in which its electrons may reside. After leaving the atom, upon ionization, the electron has 3 translational degrees of freedom. The atom is left with fewer degrees of freedom because the lost electron will no longer occupy its energy states and the overall result is that the average number of degrees of freedom per particle in the system has decreased.

If we choose to fit the data with exponentials of the form

$$Ae^{-\varepsilon/\varepsilon_2}$$

then our method leads us to the following form for the equation of state:

$$P = (\gamma - 1)\,\rho\,\varepsilon$$

$$\gamma - 1 = \left\{a + b\,e^{-\varepsilon/\varepsilon_1} f_1 + c\,e^{-\varepsilon/\varepsilon_2}(1 - f_1) + d\,e^{-\varepsilon/\varepsilon_3} f_2 + g\,f_3\right\} \frac{\rho}{\rho_o}^{a(\varepsilon)}$$

$$a(\varepsilon) = a_1 f_1 + a_2 (1 - f_1)(1 - f_2) + a_3 (f_2)$$

(We might expect the density spread to be different for each regime.)

$$a_1 = \beta_1 \log \varepsilon; \quad a_2 = \beta_2 \log \varepsilon; \quad a_3 = \beta_3$$

The "switches" are given by

(Oxygen) $$f_1 = \frac{1}{e^{\left(\frac{\varepsilon - \varepsilon_{O_2 \to 2O}}{\Delta\varepsilon_{O_2 \to 2O}}\right)} + 1}$$

(Nitrogen) $$f_2 = \frac{1}{e^{\left(\frac{\varepsilon - \varepsilon_{N_2 \to 2N}}{\Delta\varepsilon_{N_2 \to 2N}}\right)} + 1}$$

(Electrons) $$f_3 = \frac{1}{e^{\left(\frac{\varepsilon_e - \varepsilon}{\Delta\varepsilon_e}\right)} + 1}$$

This is still not complicated enough to give a close description, since each transition energy and width decreases with decreasing density. This density dependence was represented by

$$\varepsilon_{0_2 \to 20} = \varepsilon_0 \left(\frac{\rho}{\rho_o}\right)^{\delta} \qquad \text{etc. and}$$

$$\Delta\varepsilon_{0_2 \to 20} = \Delta\varepsilon_0 \left(\frac{\rho}{\rho_o}\right)^{\eta} \qquad \text{etc.}$$

The constants were evaluated by a very straightforward technique: guess values, plot curves, guess new values. Toward the end, the curves were computed by machine, but the same technique was followed. After many tedious attempts, each coming a little closer, it was decided to stop, call this an interim equation of state, and continue with more dignified techniques. The results of the program to date indicate that the approach is worthwhile. Rather than list values for each constant (which will probably change later) we list a subroutine (appendix I) in FORTRAN which will produce $(\gamma-1)$ with an error generally from 0-2 percent with occasional increases to 5 percent. The tabulated and fitted values of $(\gamma-1)$ are given in figure 2. The equations with numbers appear in appendix II. Temperatures above 1.5 ev were not given much consideration, since radiation transport influences things above that temperature, and our planned application is for "simple" hydrodynamics only. It may be possible to continue the description of regime IV to infinite energy by using a TFD equation of state.

Further applications of this fit are numerous. With this equation of state, one can use SHELL for fireball computations and probably believe the temperatures. The same form may hold for other gases and vapors.

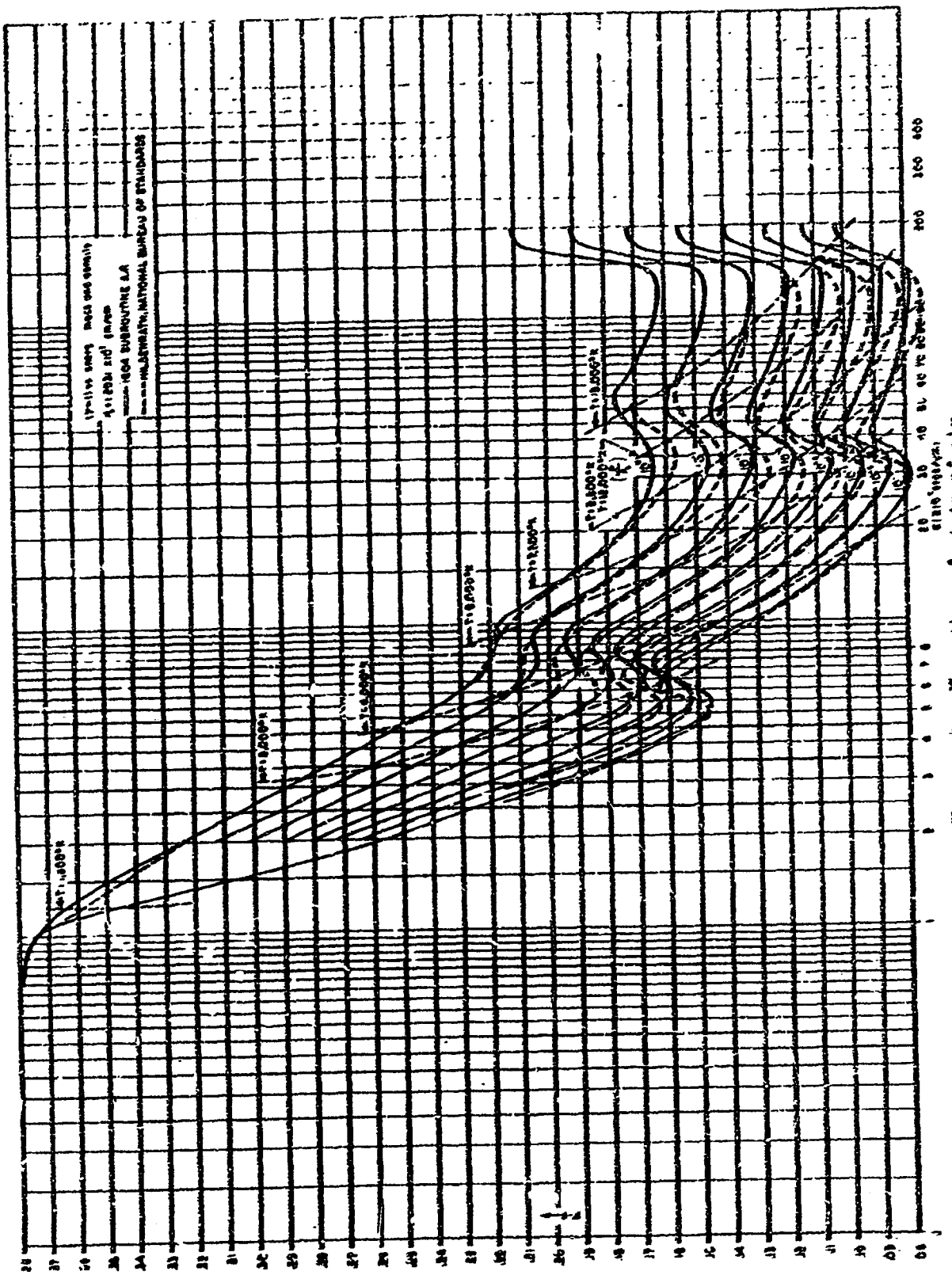


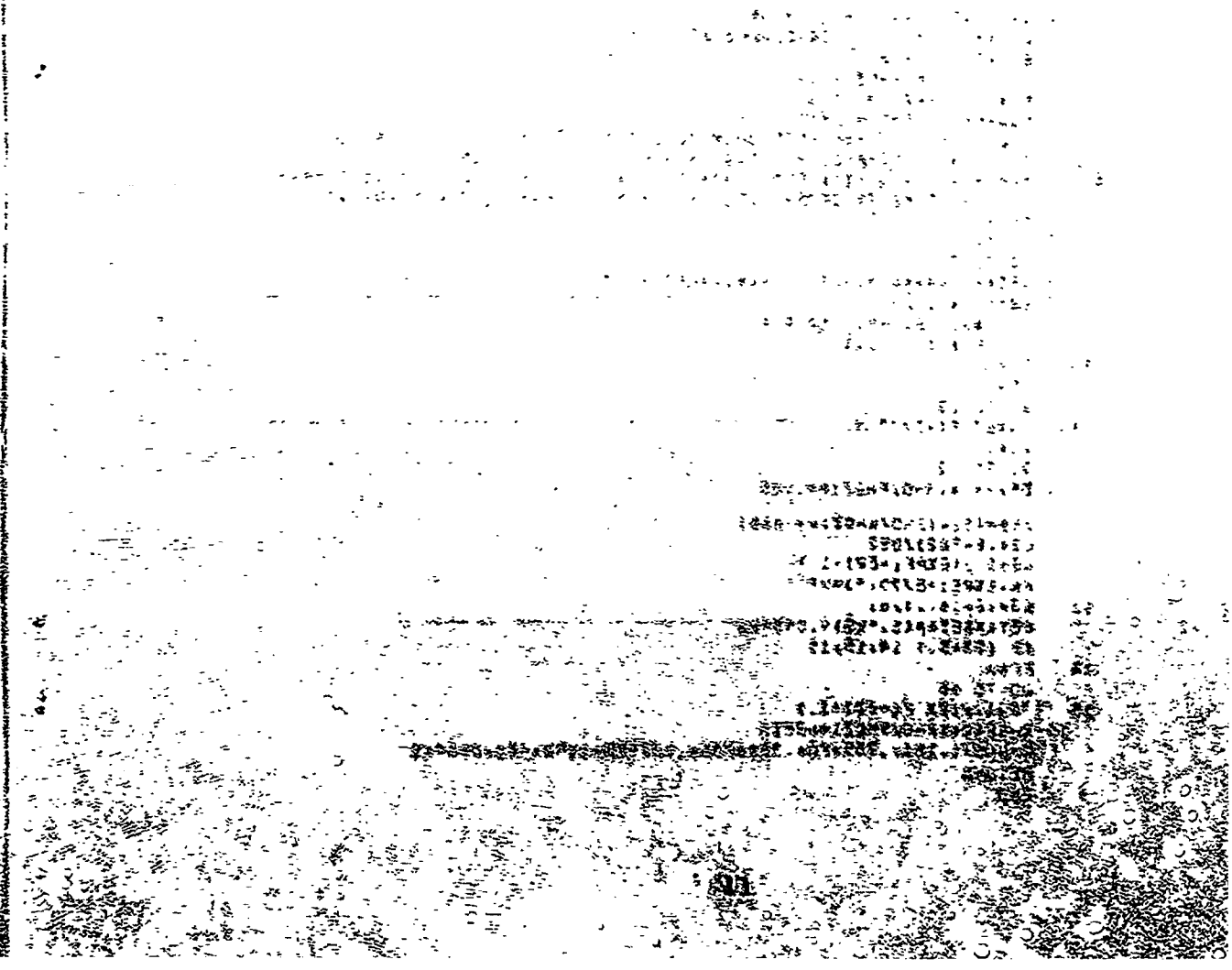
Figure 2. Equation of state of air.

Lt. J. D. Garcia has suggested that altering the energies of transition may account for nonequilibrium effects in dissociation as the fireball expands rapidly. This seems quite possible, once it can be determined how to compute the new transition energy. Techniques to determine the coefficients from theoretical methods (as opposed to curve-fitting) may uncover new freedom in generating equations of state for other gases.

Finally, the continuation of this work to include equations of state for earth, fire, and water will allow calculations for all possible substances.

Appendix I

A LISTING OF THE FORTRAN SUBROUTINE AIR



```
      SUBROUTINE AIM
      COMMON  RHO,E,RHO2,GMONE,E2
C
C     SEMI-PHYSICAL FIT TO THE EQUATION OF STATE OF AIR
C
C        TEMPERATURES FROM .025 TO 1.0 ELECTRON VOLTS
C        DENSITIES FROM 10**-2 TO 10**(+3) NORMAL DENSITY
C        PRESSURE = (GAMMA-1.)*RHO*E, WHERE GAMMA IS A FUNCTION OF
C         DENSITY AND ENERGY
C     RHO = MATERIAL DENSITY
C     RHO2 = 1.293E3 MEGAGRAMS/CUBIC KILOMETER, IN THE UNITS OF THE
C         PROBLEM
C     E = ENERGY/RHO**3
C     E2 = 1 JERK/MEGAGRAM, IN THE UNITS OF THE PROBLEM
C     GMONE = GAMMA MINUS ONE
C     MAKE E POSITIVE IF NEGATIVE, AND CONVERT TO JERKS/MEGAGRAM
      E=ABSF(E)/E2
C     THE ENERGY AT WHICH OXYGEN AND NITROGEN DISSOCIATE IS A
C     FUNCTION OF DENSITY
      E1=(RHO+5.)/.975
C     THE FERMI-DIRAC FUNCTION IS ONLY COMPUTED WITHIN 9.*DELTA E OF
C     EACH TRANSITION, OTHERWISE IT IS ONE OR ZERO
      IF (ABSF(E1)-9.) 7,4,4
    4 IF (E1) 5,5,6
    6 FO=EXPF(-E/4.48)
      FO1=FO
      WS=1.
      GO TO 8
    5 FO=0.
      FO1=EXPF(-E/6.63)
      WS=0.
      GO TO 8
    7 DE1=.975*(RHO/RHO2)**.89
      EE1=8.5+.357*LOGF(RHO/RHO2)/2.3026
      E1=(E1-E)/DE1
      WS=1./(EXPF(-E1)+1.)
      FO=EXPF(-E/4.48)*WS
      FO1=EXPF(-E/6.63)*(1.-WS)
C     THE DENSITY DEPENDENCE ONLY OCCURS ABOVE E=1., AND IT IS OF
C     THE FORM (RHO/RHO2)**(CONSTANT*LOG(E)).  THE CONSTANT
C     MAKES A TRANSITION FROM .048 TO .029 AS THE OXYGEN DISSOCIATES
C     AND THE DENSITY SPREAD BECOMES CONSTANT BEYOND THE THIRD PEAK
    8 IF(E-1.) 1,1,2
    1 BETA=0.
      GO TO 3
    2 BETA=(.048*WS+.029*(1.-WS))*LOG(E)/2.3026
    3 E2=(E*48.)/3.
      IF (ABSF(E2)-5.) 12,9,9
    9 IF (E2) 10,10,11
   10 FN=0.
      WS0=0.
      GO TO 13
   11 FN=EXPF(-E/29.9)
      WS0=1.
      GO TO 13
   12 DE2=4.*(RHO/RHO2)**.885
      EE2=45.*(RHO/RHO2)**.8157
      E2=(E-EE2)/DE2
      WS=1./(EXPF(-E2)+1.)
      FN=EXPF(-E/29.9)*WS
   13 E3=(E-164.)/8.
      BETA=BETA*(1.-WS)+.049*WS
      IF (E3+9.) 14,15,15
   14 FE=0.
      GO TO 16
   15 FE=1./(EXPF(-E3)+1.)
   16 RHOFAC=(RHO/RHO2)**BETA
      GMONE=(1.101+.295*FO+.200*FO1+.127*FN+.138*FE)*RHOFAC
      RETURN
      END
```

Appendix II

The equation with the present numbers:

$$\gamma - 1 = \left\{.161 + .255\, e^{-\varepsilon/4.46} f_1 + .280\, e^{-\varepsilon/6.63}(1 - f_1) + .137\, e^{-\varepsilon/25.5} f_2 + .050\, f_3\right\} \left(\frac{\rho}{\rho_o}\right)^{\alpha(\varepsilon)}$$

$$\alpha(\varepsilon) = .048\, f_1 \log_{10} \varepsilon + .032\,(1 - f_1)(1 - f_2) \log_{10} \varepsilon + .045\, f_2$$

$$f_1 = \frac{1}{e^{\frac{\varepsilon - \varepsilon_1}{\Delta\varepsilon_1}} + 1} \qquad \varepsilon_1 = 8.5 + .357 \log_{10} \left(\frac{\rho}{\rho_o}\right)$$

$$\Delta\varepsilon_1 = .975 \left(\frac{\rho}{\rho_o}\right)^{.05}$$

$$f_2 = \frac{1}{e^{\frac{\varepsilon_2 - \varepsilon}{\Delta\varepsilon_2}} + 1} \qquad \varepsilon_2 = 45. \left(\frac{\rho}{\rho_o}\right)^{.0157}$$

$$\Delta\varepsilon_2 = 4.0 \left(\frac{\rho}{\rho_o}\right)^{.085}$$

$$f_3 = \frac{1}{e^{\frac{\varepsilon_3 - \varepsilon}{\Delta\varepsilon_3}}} \qquad \varepsilon_3 = 160.$$

$$\Delta\varepsilon_3 = 6.$$

REFERENCES

1. Hilsenrath, Klein, and Woolley, Tables of Thermodynamic Properties of Air Including Dissociation and Ionization from 1,500°K to 15,000°K, NBS, AEDC TR 59-20, December 1959.

2. Gilmore, F. R., Equilibrium Composition and Thermodynamic Properties of Air to 24,000°K, RAND, RM-1543, 24 August 1955.

DISTRIBUTION

No. cys	
	AFWL, Kirtland AFB, N Mex
15	(WLRP)
3	(WLRM)
1	(WLRJ)
1	(WLRB)
1	(WLRS)
5	(WLL)
1	Director, USAF Project RAND, via: Air Force Liaison Office, The RAND Corporation, 1700 Main Street, Santa Monica, Calif
1	Director, Los Alamos Scientific Laboratory (Helen Redman, Report Library), P. O. Box 1663, Los Alamos, N Mex
1	University of California Lawrence Radiation Laboratory (Technical Information Division), P. O. Box 808, Livermore, Calif
1	General Atomic, Division of General Dynamics Corporation, P. O. Box 1608, San Diego 12, Calif
1	Official Record Copy (WLRPT, Capt Atkins)